SPEAM-II EXPERIMENT FOR THE MEASUREMENT OF STRATOSPHERIC NO₂, O₃ AND AEROSOLS

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ABSTRACT

Following the success of the Sunphotometer Earth Atmosphere Measurement (SPEAM-I) experiment, a more involved experiment was developed to fly as part of the second set of Canadian Experiments (CANEX-2) which will fly on the US Space Shuttle in the fall of 1992. The instrument complement includes an IBM-PC compatible control computer, a hand-held diode array spectrophotometer, and an interference-filter, limb imaging radiometer for the measurement of the atmospheric airglow. The hand-held spectrometer will measure nitrogen dioxide, ozone and aerosols. The limb imaging radiometer will observe emissions from the $\mathrm{O_2^{1}\Delta}$ and $\mathrm{O_2^{1}\Sigma}$ airglow bands. Only the spectrophotometer will be discussed here.

1.0 INTRODUCTION

Recent advances in understanding the processes which control the chemistry of the stratosphere have pointed to the need for an increase in the scope of space-based, upper-atmospheric monitoring systems. In particular, the measurement of nitrogen oxides and ozone on a global scale is essential for monitoring the effects of anthropogenic pollutants and the impact of volcanic aerosols on the ozone layer. For this reason, a number of spaced-based instrument initiatives have been made during the last two decades; for example: the Total Ozone Mapping Spectrometer (TOMS), the Stratospheric Aerosol and Gas Experiment (SAGE), the Upper Atmospheric Research Satellite (UARS), the Global Ozone Monitoring Experiment (GOME), and the EOS program.

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One problem which will always exist for satellite systems is the difficulty of making a long-term verification and calibration of their instrumentation. To date, this calibration function has been carried out using comparisons between ground-based observations and the data collected by satellite. Indeed, much of the early work on the remote sensing of temperature used comparison data as the basis of the retrieval algorithms.

Physical models are also used to retrieve information about the atmosphere from measurements made by satellite systems, but the ultimate validation of the whole retrieval process has still rested on the comparison of the satellite measurements with those made using other techniques. For example, the Total Ozone Mapping Spectrometer (TOMS) data have been compared to the global ozone data set measured by the ground-based Global Ozone Observing System. The differences in the measurement methods, and the lack of exact time and space coincidence in the two measurement sets provide a limit to the amount of information available concerning the physical calibration of

the satellite instrumentation. In fact, this is generally true for any measurement system.

The SunPhotoSpectrometer (SPS) will be pointed at the sun from the mid-deck of the Space Shuttle, and will make measurements of the sunlight transmitted to the instrument through the atmosphere as the sun sets because of the orbital motion of the spacecraft (solar occultation measurements). Limb scanning measurements, and measurements of the light backscattered by the Earth's atmosphere and reflected from its surface will also be attempted. These data will be analyzed to produce altitude profiles of O3, NO2 and aerosols.

2.0 INSTRUMENTATION

Two instruments and a control computer have been developed in the laboratory at the Atmospheric Environment Service of Canada (AES) and will be operated by the next Canadian Payload Specialist to fly on the US Space Shuttle. The flight is expected to take place in the fall of 1992. The instruments to be flown are the Airglow Imaging Radiometer (AIR) and the SunPhoto-Spectrometer (SPS). The AIR is a limb-imaging radiometer based on a 16-element germanium detector array.

The SPS is a Reticon diode array spectrometer based on a concave, holographic diffraction grating. The entrance slit is 50 microns wide, and the aperture is f/2. The instrument is designed to have a free spectral range of 400-800 nm in the first order and 200-400 nm (UV) in the second order. A filter wheel is mounted in the space between the field lens and the entrance slit. The filters are used to reject unwanted light and to select the order in which the diffraction grating is used. The entrance lens has a focal length of 25 mm, so the field-of-view (FOV) of the instrument ls approximately 0.1 degrees.

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The spectrometer is powered by an internal alkaline battery pack which can operate it for up to 6 hours. The instrument is 16 x 20 x 11 cm and weighs 2.9 kg including batteries.

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Because it is difficult to point an instrument manually to an accuracy of 0.1°, but it is possible to point one to better than ±1° [McElroy et al., 1991], the spectrometer is equipped with a mirror which scans the instrument field of view rapidly through a range of ±0.75° either side of the direction determined by the operator's aiming of the instrument. The 'slices' of the solar disc which are observed will be postprocessed to yield spectra which can be associated with an identifiable point near the centre of the solar disc. This technique is similar to that used on the SAGE satellite instrument [McCormick et al., 1979].

The SPS is pointed using information

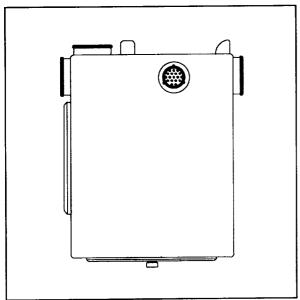


Figure 1 This plan view of the SPS shows the sighting ports at the upper left and the entrance window to the upper right. The instrument is 16 x 20 x 11 cm and weighs 2.9 kg including batteries.

presented to the operator in the form of a small solar image on a diffusing screen. The light which forms the image passes through a beam splitter which reflects 80% of the light into the instrument and passes about 10% on to the sight imaging system. The lens system projects an image of the sun and of an embedded cross-hair onto two screens, either of which can be used to point the instrument (Figure 1). There is also a coarse 'peepsight' mechanism for the initial setup of the instrument.

The spectrometer control software is started before the observation period begins, data are collected for a period of time, and then the computer is stopped. Using a cursor on a graphical presentation of the data collected, the operator can select the section which is of interest and discard the beginning and end of the sequence where the instrument was being set up, and the computer being halted. The data are stored in credit-card-sized electrically-erasable memory cards which will be returned to the ground after the flight.

While the instrument has been designed primarily to make measurements from the Space Shuttle mid-deck, other applications for the device are envisioned; including ground-based turbidity monitoring, aircraft-based measurements of the global radiation field at high altitudes, and growth into a satellite instrument. For this reason, attention has been given to the robustness of the design and to the compensation of the instrument's properties for temperature changes.

3.0 CHARACTERIZATION

When determining absorption amounts using high resolution spectral data, the amounts are found essentially by making use of those variations with wavelength which each absorbing material uniquely contributes to the absorption spectrum. The observed spectrum is fitted as the sum of the effect of each absorber contributing to the net optical depth, together with an estimate of the incident spectrum [Solomon et al., 1987]. Because

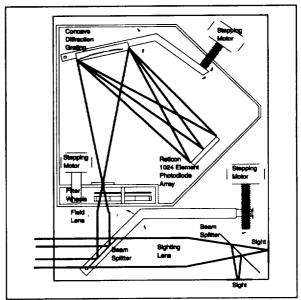


Figure 2 The optics of the SPS in schematic form. Light enters at the lower left and is reflected upward into the spectrometer by the scanning beamsplitter. Motors operate the scanner, the entrance filter wheel, and the grating tilt.

of the presence of strong, narrow Fraunhoffer lines in the solar spectrum, it is necessary to maintain an extremely high-precision wavelength calibration. This is required so that the absorption measurements made at any given time can be accurately analyzed using a reference spectrum made at a different time or even by a different instrument.

There are two instrumental sources for errors in this analysis. One of these is the misassignment of wavelengths, which was described above. The other is the effect which changes in the instrument slit function will contribute. This will affect the matching of the Fraunhoffer lines in the reference spectrum to those in an observation, and will also contribute to an uncertainty in the absorption coefficients appropriate for a given absorber due to the precise slit function of the instrument at the time of the observations.

If the slit function of the instrument can be stabilized to a high degree, shifting and stretching operations can be used to mathematically calibrate the wavelength scale of an observed spectrum to agree with a particular (calibrated) reference spectrum and the absorption coefficient spectra. Therefore, the SPS design includes careful stabilization of the slit function with respect to temperature (i.e. the focus of the spectrometer) but does not attempt to stabilize the dispersion of the instrument to a high degree.

Figure 2 shows the layout of the SPS. The spectrometer is constructed mostly of 6061-T6 aluminum alloy to have good strength, low weight and easy machinability of the instrument parts. To stabilize the focus of the instrument against temperature changes, the diode array detector subsystem is positioned with respect to the diffraction grating and entrance slit by a mount containing both plastic (ABS) and invar. This mount makes the detector subassembly move toward the grating as a function of temperature, thereby compensating for a general growth of the aluminum

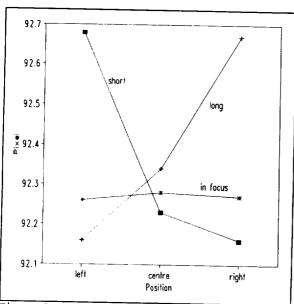


Figure 3 Focusing curves for the detector system are presented in this figure. The centre curve shows the spectral spreading due to coma because of the large aperture (f/2) of the instrument.

structure of the spectrograph as a function of temperature.

The growth of the instrument with temperature, in the absence of this compensation, would cause the image on the detector to go out of focus as the focal plane of the grating moved toward the grating surface (as the entrance slit moves away). This motion is tracked by the compensated detector subsystem. As the focal surface moves, the dispersion will also change. This means that the compensated instrument will maintain its slit function as temperature changes, but that the wavelength dispersion of the system will still change. This must be compensated in the spectral analysis algorithm as discussed earlier.

The performance of the instrument in terms of its wavelength stability and its focus behaviour were investigated using a spectral line finder (provided by A. Goldman, University of Denver). The algorithm uses search criteria to identify either emission or absorption lines (as desired) and then predicts the intensity and the centre wavelength of a line using a quadratic interpolation based on the intensity values of 3 consecutive points. Testing has shown that, at reasonable signal levels, the instrument and line finder show a consistency of about 0.01 pixel. Figure 3 shows the performance of the instrument as a function of temperature. The focus of the instrument is estimated by plotting the position which the line finder assigns an emission line as a function of whether the light enters along a pencil of rays near the centre of the FOV, or near the left or right edges.

If the spectrograph is out of focus, the behaviour of the line positions will be as shown by 'short' or 'long' curves shown in Figure 3. If the rays of light come to a focus short of the detector array, it means that rays from the opposite sides of the FOV will cross before reaching the detector and will lie to either side of the central ray. If the grating is moved enough that the focus falls beyond the detector, the relative positions of the edge rays will reverse. This is shown as the long

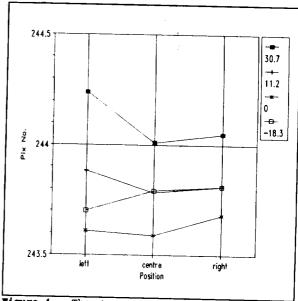


Figure 4 The temperature dependence of the instrument focus is presented. There is less than a 0.2 pixel (0.1 nm) change in focus over a 40 degree C range.

curve in Figure 3. An ideal instrument in perfect focus will have all the rays within the field of view converging at the same lateral position on the focal plane.

focal plane.

In practice, optical instruments suffer from aberrations in their image forming properties. The first asymmetrical aberration is coma. Coma is evidenced in the focusing test by the fact that, at best focus, the rays from the two edges of the field of view lie to the same side of the central ray focal position. This sets a limit on the ultimate resolution of the system. Figure 3 shows the best focus of the instrument as the 'in-focus' curve.

The behaviour of the focus of the spectrograph as a function of temperature was investigated and is shown in the plots presented as Figure 4. These show the result of stabilizing the instrument focus against temperature changes. It can be seen that the worst case impact on the slit function is a change in the full-width-at-half-maximum (FWHM) of the order of 0.2 pixel, while the FWHM as determined by the instrument geometry (entrance slit width) is 2 pixels.

The instrument includes stepping motors which move the filter wheel and aperture disc, scan the instrument field of view, and tilt the diffraction grating approximately 1 full resolution element (2 pixels) in very small steps; about 1/20 of a pixel. This last motor is included for two purposes. One application is in the characterization of the instrument. Scanning the grating in very small steps while observing an emission line source allows the determination of the instrument slit function with greater precision. Scanning in small steps while preparing a Langley plot allows the creation of an oversampled spectrum for use as a reference in the analysis of observational data. The use of a reference spectrum which includes many more elements at closer spacing than the detector physically possesses eliminates the aliasing problem which would result if the solar spectrum were interpolated in the data analysis procedure

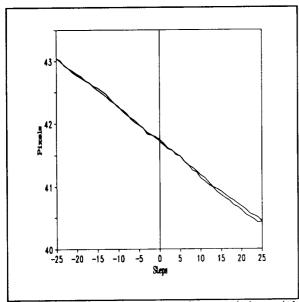


Figure 5 This plot shows the precision with which the line-finder and the grating microstepping adjustment system operate. The RMS variation of the adjusting system is 0.02 pixels (0.01 nm).

using only 2 pixels per resolution element.

This aliasing problem exists because the solar spectrum is not properly band-limited and when an observed spectrum or reference solar spectrum is interpolated to bring them into wavelength alignment the interpolation routine may not give the correct value at intermediate wavelengths. The higher sampling rate available using mechanical scanning provides a reference spectrum which can be properly interpolated to match a particular observed spectrum.

Since the Langley analysis procedure is carried out under the best of observing conditions, and can include a large amount of data, the features of the reference spectrum can be much better determined than those of any single, observed spectrum. This means that the propagation of noise in the interpolation process will be greatly reduced.

The performance of the grating tilting mechanism is shown in Figure 5. The performance testing was done by tracking the motion of mercury emission lines as the grating motor was moved. Fitting a least squares line to the successive step positions allows an estimate of the precision of the tilting drive motion. The RMS difference between the calculated step positions and the observed line positions was calculated to be 0.023 pixels (0.012 nm) as compared to an error (calculated above) of 0.01 pixels (0.005 nm) for the line finder alone.

Figure 6 gives an indication of the performance of the instrument. The upper curve is a spectrum of the sun taken at the Mauna Loa Observatory in February 1992. The middle one is a wavelength reference spectrum (mercury discharge lamp), and the lowest one is a dark reference spectrum which is used to correct for the dark offset of the system in the analysis of the data. The spectrum covers the range from 400-800 nm with a resolution of about 1 nm. The analysis of two spectra taken close together in time has shown that the instrument can provide photometric information

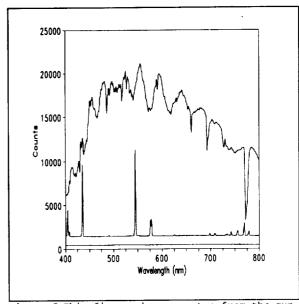


Figure 6 This figure shows spectra from the sun, a mercury arc and the detector background. Etalon fringes from the passivating layer on the detector are apparent in the solar spectrum.

with a precision better then 0.1%.

4.0 CONCLUSIONS

The use of modern array detectors offers the potential for extremely precise photometry under physical conditions which preclude the use of conventional, low-noise scanning spectrometers. It is hoped that the successful use of the SPS onboard the US Space Shuttle will point the way for the development of small hand-held, precise instruments for use in monitoring the Earth's atmosphere and the calibration of sensors permanently stationed in space.

5.0 ACKNOWLEDGEMENTS

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